

Supporting Information

The use of mass spectrometry imaging to predict treatment response of patient-derived xenograft models of triple-negative breast cancer

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Figure S-1

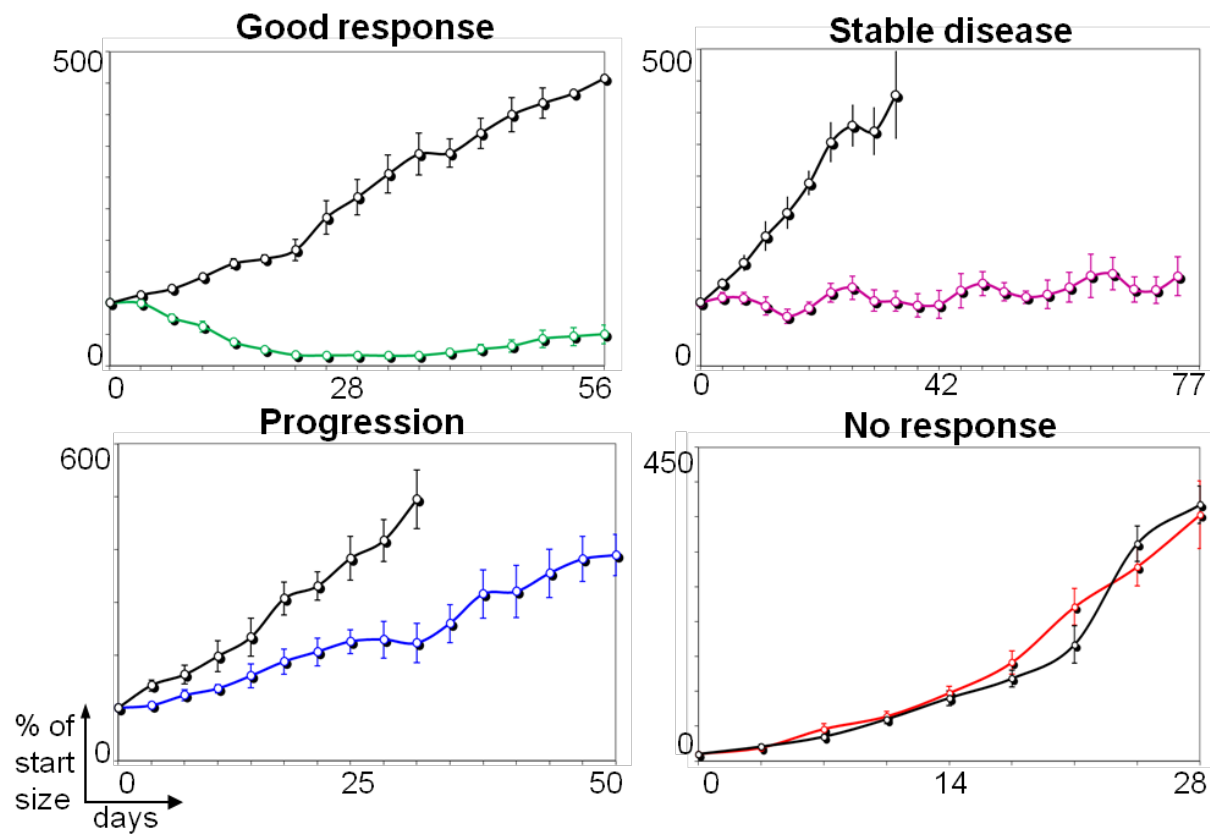


Figure S-1. Response to cisplatin. Black lines show growth of untreated controls. In all graphs, the y-axis depicts tumor size (% of start size), and the x-axis depicts the days after start of treatment. Representative examples for each response are shown.

Figure S-2

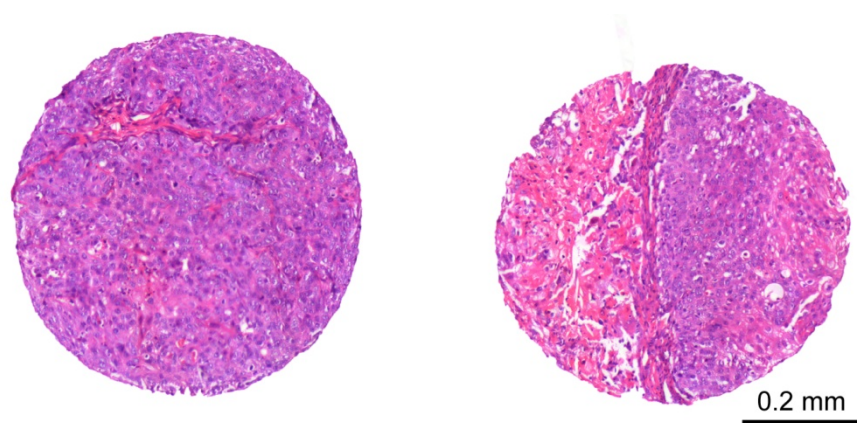


Figure S-2. Examples of tissue cores of a TNBC PDX model. On the left an example of a homogeneous core with a tumor cell content of 90% is shown. On the right a histologically heterogeneous core of the same tumor containing stromal regions (pink) is shown.

Figure S-3

a)

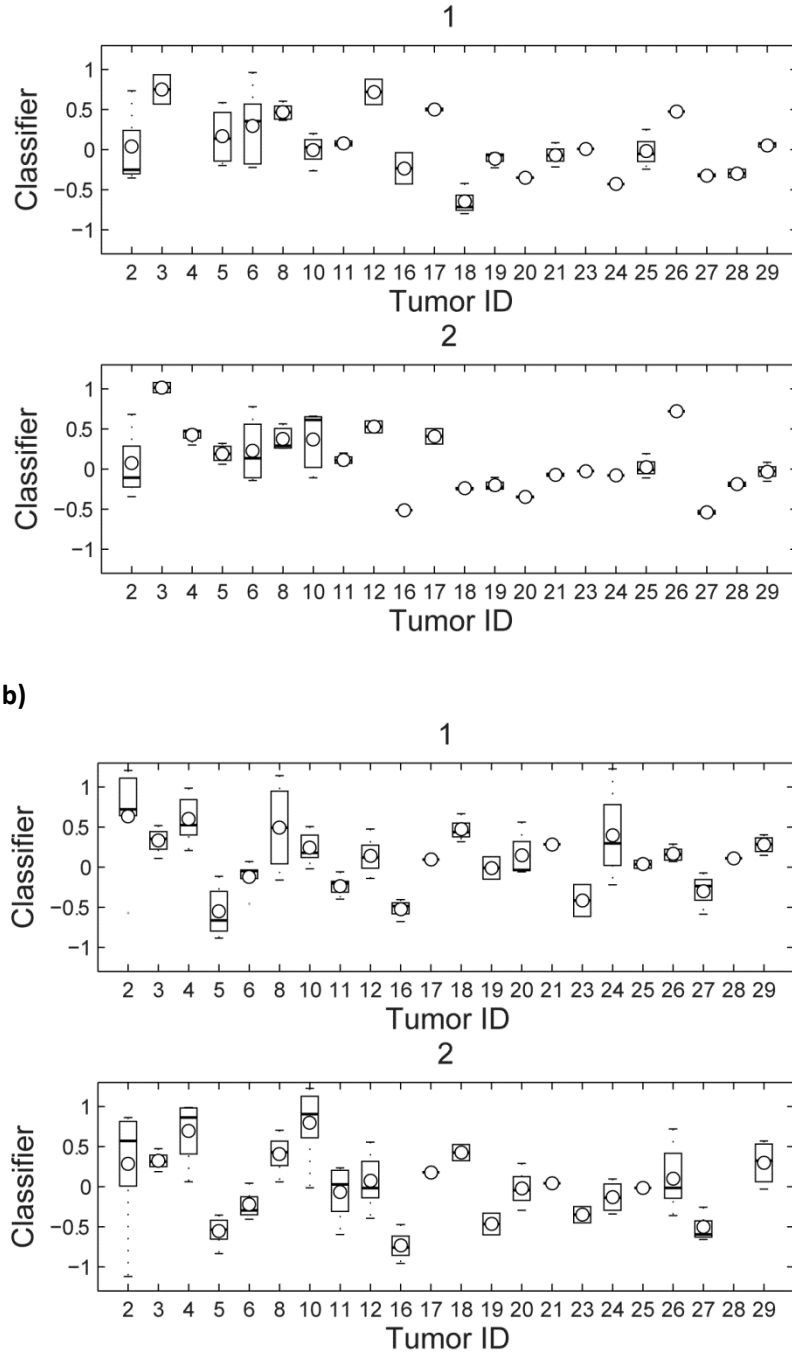


Figure S-3. Box plots for the cross-validation of (a) TMA1 and (b) TMA2 from Figure 2 for each measurement separately. Overall, the cross-validation scores for each tumor model were similar between measurements of consecutive TMA sections (here named 1 and 2).

Figures S-4 and S-5

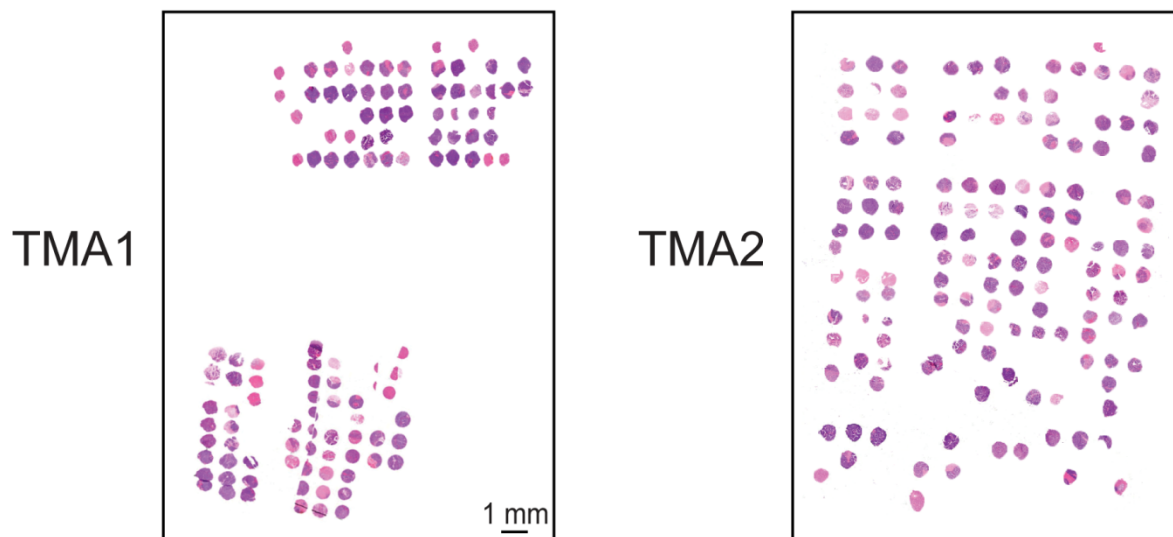


Figure S-4. Optical images of H&E stained TMA sections. All cores on the TMAs are shown, including control cores and cores from non-TNBC PDX models, which were not included in this study.

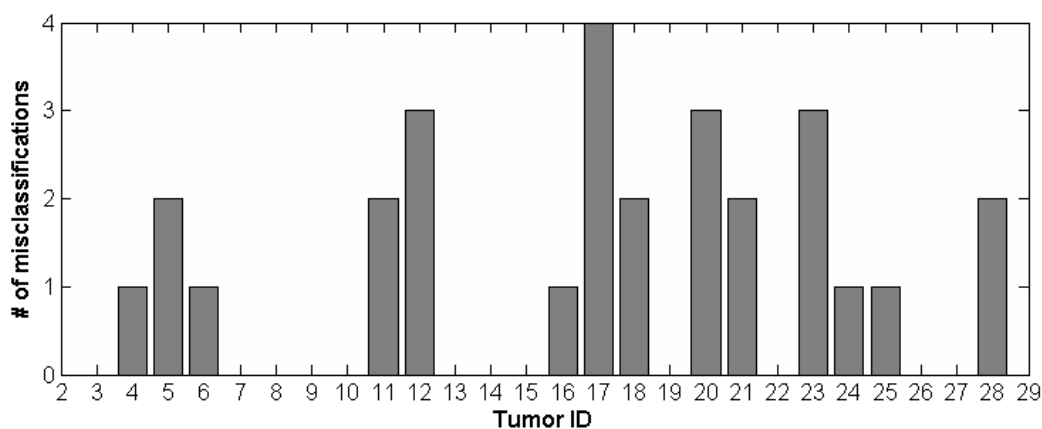


Figure S-5. The total number of misclassifications per PDX model. The misclassifications of the cross-validations and the reproducibility tests are summed. The four most often misclassified models, namely 12, 17 20 and 23 had all shown an intermediate response phenotype in the treatment response experiments.

Figure S-6 and Table S-1

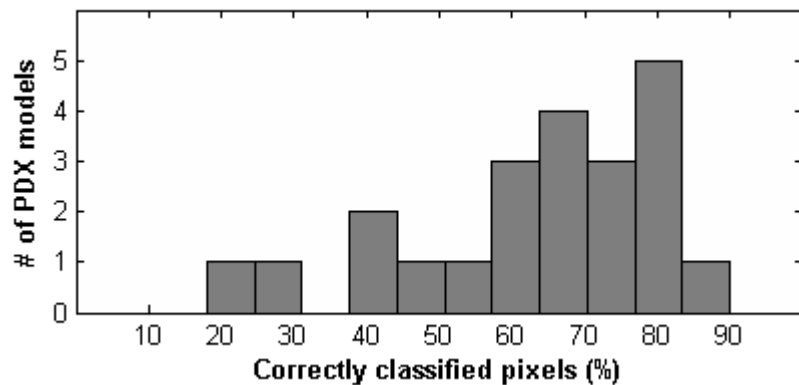


Figure S-6. Distribution of the percentage of correctly classified pixels per PDX model. The percentages are averaged over all predictions per tumor model presented in Table 3.

Table S-1. Samples used for construction of the classifiers based on the full datasets of TMA1 and TMA2. PCA-LDA was performed using 32 and 39 PCs for the TMA1 and TMA2 based classifier, respectively.

Dataset	Response class	No. of tumor models	No. of tissue cores
TMA1	Responder	12	85
	Non-responder	10	56
TMA2	Responder	12	173
	Non-responder	10	113

Table S-2

Table S-2. Classification results for the double cross-validations and the reproducibility tests using the complete data sets: no selection of regions with high tumor cell content was made.

Dataset		Cross-validation		Reproducibility test	
TMA1	Tumor model	17/22	(77%)	20/22	(91%)
	Tissue core	94/141	(67%)	114/141	(81%)
TMA2	Tumor model	14/22	(64%)	19/22	(86%)
	Tissue core	165/254	(65%)	190/254	(75%)